57. Monte Carlo Simulations for Systems of Hard Repulsive Objects(poster presentation,Soft Matter as Structured Materials)

AUTHOR(S):

KODA, Tomonori; NISHIOKA, Akihiro; IKEDA, Susumu

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Monte Carlo Simulations for Systems of Hard Repulsive Objects

Faculty of Engineering, Yamagata University
Tomonori KODA[1], Akihiro NISHIOKA, and Susumu IKEDA

球，冠球円柱，カットスフェア，冠球円盤と，三角分割で表現できる剛体微粒子について，それらが凝集し，平衡状態において形成する構造を明らかにするための汎用シミュレーターを開発中である．そのシミュレーターの紹介，および，いくつかの課題に適用した結果を発表する．

Theories and simulations have shown that repulsive anisotropic particles show various types of liquid crystal structures. Nematic structure is observed in systems of hard ellipsoids of revolution, hard spherocylinders, and hard cutspheres. Smectic structure is observed in systems of hard spherocylinders. Columnar structure is observed in systems of cut spheres.

For development of the study of hard particles, we are now building a simulation software that generates equilibrium structure of hard repulsive particles of general shapes. The shapes of particles include sphere, spherocylinder, cutsphere, spheroplatelets, and shapes that is expressed by triangulation. The simulation software performs isobaric Monte Carlo simulation of these hard bodies.

In this presentation, we show results obtained using the software. As an example, Figure 1 shows a snapshot of simulation of binary mixture of hard spheres and hard spheroplatlets. Phase separation of spheres and spheroplatelets is observed. In the structure of spheroplatelets, local column formation is noticed.

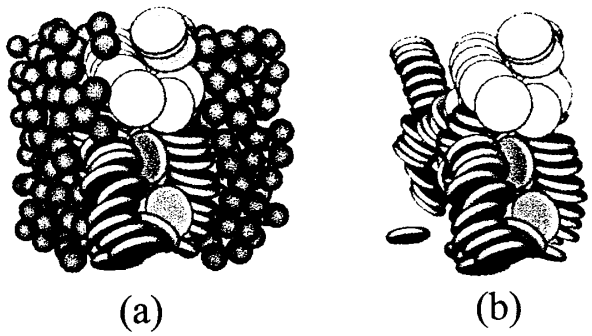

Figure 1: Phase separation between spheroplatelets and spheres. Spheres in (a) is removed to show structures (b) of spheroplatelets.

[1]E-mail: koda@yz.yamagata-u.ac.jp